search for $H_2{}^{17}O$ solutions


```
=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 17:27:52 ON 21 JUL 2003
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FILE COVERS 1907 - 21 Jul 2003  VOL 139 ISS 4
FILE LAST UPDATED: 20 Jul 2003  (20030720/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d que l32

L1         1299 SEA FILE=REGISTRY ABB=ON  PLU=ON  17O
L2           20 SEA FILE=REGISTRY ABB=ON  PLU=ON  L1 AND "WATER"
L3           17 SEA FILE=REGISTRY ABB=ON  PLU=ON  L2 AND " WATER-17O"
L4            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L3 AND H2O/MF
L5            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND NC=1
L6            2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 NOT T/ELS
L7            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  15587-57-2 H2 17 O
L8          169 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L6 OR L7)
L25          56 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND (NMR OR MAGNETIC)/OBI
L32           9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND TISSUE 9 cites

=> d que l33

L1         1299 SEA FILE=REGISTRY ABB=ON  PLU=ON  17O
L2           20 SEA FILE=REGISTRY ABB=ON  PLU=ON  L1 AND "WATER"
L3           17 SEA FILE=REGISTRY ABB=ON  PLU=ON  L2 AND " WATER-17O"
L4            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L3 AND H2O/MF
L5            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND NC=1
L6            2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 NOT T/ELS
L7            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  15587-57-2
L8          169 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L6 OR L7)
L25          56 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND (NMR OR MAGNETIC)/OBI
L26           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND COMPOSITION
L27           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND (BOLUS OR LIPOSOM?)
L28           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND DIAGNOS?
L29           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND ORGAN
L30           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND DISEASE
L31           2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L25 AND (AMINO ACID)
L33           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L26 OR L27 OR L28 OR L29 OR
                 L30 OR L31) 8 cites

=> d que l74
```

nc = # components
T = Tritium
els = element symbol
obi = all search fields except for abstract

```
L1          1299 SEA FILE=REGISTRY ABB=ON  PLU=ON  170
L2            20 SEA FILE=REGISTRY ABB=ON  PLU=ON  L1 AND "WATER"
L3            17 SEA FILE=REGISTRY ABB=ON  PLU=ON  L2 AND " WATER-170"
L4             4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L3 AND H2O/MF
L5             4 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND NC=1
L6             2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 NOT T/ELS
L7             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  15587-57-2
L8           169 SEA FILE=HCAPLUS ABB=ON   PLU=ON  (L6 OR L7)
L11            2 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L8 AND (PHARMA? OR DRUG)
L15        44081 SEA FILE=HCAPLUS ABB=ON   PLU=ON  DIAGNOSIS+PFT/CT
L16            2 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L15 AND L8
L17            1 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L8(L)(DGN)/RL
L19            5 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L8 AND SOLVENT
L20           19 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L8 AND SOLUTION
L21           18 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L20 NOT L19
L22            2 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L21 AND HYDRATION NUMBER/OBI
L23         4954 SEA FILE=HCAPLUS ABB=ON   PLU=ON  IMAGING AGENTS+PFT,NT/CT
L24            3 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L23 AND L8
L74            6 SEA FILE=HCAPLUS ABB=ON   PLU=ON  L11 OR (L16 OR L17) OR L22 OR
                  L24
```

6 cites

PFT = old, new & "used for" terms

CT = controlled terminology

DGN = diagnosis

RL = role

NT = narrower term

```
=> s l32-33 or l74

L103        13 (L32 OR L33) OR L74

=> file wpix

FILE 'WPIX' ENTERED AT 17:27:55 ON 21 JUL 2003
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FILE LAST UPDATED:          19 JUL 2003      <20030719/UP>
MOST RECENT DERWENT UPDATE:     200346        <200346/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> NEW WEEKLY SDI FREQUENCY AVAILABLE --> see NEWS  <<<

>>> SLART (Simultaneous Left and Right Truncation) is now
    available in the /ABEX field. An additional search field
    /BIX is also provided which comprises both /BI and /ABEX <<<

>>> PATENT IMAGES AVAILABLE FOR PRINT AND DISPLAY <<<

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES,
    SEE http://www.derwent.com/dwpi/updates/dwpicov/index.html <<<

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
    PLEASE VISIT:
 http://www.stn-international.de/training_center/patents/stn_guide.pdf <<<

>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER
    GUIDES, PLEASE VISIT:
    http://www.derwent.com/userguides/dwpi_guide.html <<<

=> d que l80

L76           75 SEA FILE=WPIX ABB=ON  PLU=ON  170 OR OXYGEN-17
L77      1190844 SEA FILE=WPIX ABB=ON  PLU=ON  H2O OR WATER
L78           26 SEA FILE=WPIX ABB=ON  PLU=ON  L76 AND L77
```

```
L80           5 SEA FILE=WPIX ABB=ON  PLU=ON  L78 AND (DRUG OR PHARMACEUT? OR
                THERAP?)  5 cites

=> d que l82

L76          75 SEA FILE=WPIX ABB=ON  PLU=ON  170 OR OXYGEN-17
L77     1190844 SEA FILE=WPIX ABB=ON  PLU=ON  H2O OR WATER
L78          26 SEA FILE=WPIX ABB=ON  PLU=ON  L76 AND L77
L80           5 SEA FILE=WPIX ABB=ON  PLU=ON  L78 AND (DRUG OR PHARMACEUT? OR
                THERAP?)
L81          21 SEA FILE=WPIX ABB=ON  PLU=ON  L78 NOT L80
L82           6 SEA FILE=WPIX ABB=ON  PLU=ON  L81 AND (YEAST OR TOMOGRAPHY OR
                PARENTERAL OR BURNS OR LIPOSOME OR MICROCLUSTER)  6 cites

=> s l80 or l82
L104         11 L80 OR L82  11 cites for permut

=> dup rem l103 l104
FILE 'HCAPLUS' ENTERED AT 17:28:37 ON 21 JUL 2003
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FILE 'WPIX' ENTERED AT 17:28:37 ON 21 JUL 2003
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PROCESSING COMPLETED FOR L103
PROCESSING COMPLETED FOR L104
L105         23 DUP REM L103 L104 (1 DUPLICATE REMOVED)  23 cites total
                ANSWERS '1-13' FROM FILE HCAPLUS
                ANSWERS '14-23' FROM FILE WPIX

=> d ibib abs ind 1-13     ind = indexing

L105 ANSWER 1 OF 23  HCAPLUS  COPYRIGHT 2003 ACS on STNDUPLICATE 1  applicants
ACCESSION NUMBER:         2000:98382  HCAPLUS
DOCUMENT NUMBER:          132:134185
TITLE:                    Drugs for therapeutic use enabling nuclear
                          magnetic resonance diagnosis by
                          scalar bond
INVENTOR(S):              Washino, Komei; Shimmura, Toshiyuki; Nakatani, Akira;
                          Fujimoto, Chieko; Tanaka, Akihiro; Seri, Shigemi;
                          Iwai, Kumiko
PATENT ASSIGNEE(S):       Nihon Medi-Physics Co., Ltd., Japan
SOURCE:                   PCT Int. Appl., 15 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.       KIND  DATE          APPLICATION NO.  DATE
     ---------------  ----  --------      ---------------  --------
     WO 2000006207     A1   20000210      WO 1999-JP3970   19990723
         W:  AU, BR, CA, CN, KR, NO, NZ, RU, US, ZA
         RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE
     JP 2000044491     A2   20000215      JP 1998-213050   19980728
     CA 2338702        AA   20000210      CA 1999-2338702  19990723
```

AU 9948005	A1	20000221	AU 1999-48005	19990723
AU 758913	B2	20030403		
EP 1101498	A1	20010523	EP 1999-931523	19990723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2001000423	A	20010124	NO 2001-423	20010124

PRIORITY APPLN. INFO.: JP 1998-213050 A 19980728
WO 1999-JP3970 W 19990723

AB **Drugs** for therapeutic use characterized by contg. a compd. which carries in its structure at least one member selected from among -17OH, -14NH and -33SH, wherein the above 17O, 14N or 33S exerts a relaxation effect on the proton bonded thereto and the relaxation effect is transported through the exchange of a proton in a vital component of a target **organ** or **tissue** by the above-mentioned proton, thus enabling detection by NMR. The effective circulation or distribution of such a physiol. acceptable therapeutic **drug** in the target **organ** or **tissue** in vivo where it is needed can be externally detected by the NMR method before the administration of a remedy to each patient or simultaneously therewith.

IC ICM A61K049-00

CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 63

ST radiopharmaceutical **diagnosis** **NMR** MRI scalar bond; infusion **liposome** radiopharmaceutical **diagnosis** **NMR** MRI

IT **Diagnosis**
(agents; **drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT Animal **tissue**
Drug delivery systems
Imaging agents
NMR (nuclear **magnetic** resonance)
Organ, animal
Positron-emission tomography
(**drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT **Amino acids**, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(**drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT **Drug** delivery systems
(infusions; **drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT **Drug** delivery systems
(**liposomes**; **drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT 257283-87-7P, D-Glucose-3-17O 257283-88-8P, D-Glucose-1-17O
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(**drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)

IT 50-21-5, Lactic acid, biological studies 50-99-7, Glucose, biological studies 4033-40-3, N-Acetyl asparagine 7727-37-9, Nitrogen, biological studies 12586-59-3, Proton 13774-92-0, Imidogen 13968-48-4, biological studies 14257-58-0, S-33, biological studies **15587-57-2**, Hydroxyl-17O 31713-49-2, Mercapto-33S
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

Indexing terms

I included the indexing terms because they cover all of the topics in the full paper. The abstract sometimes misses topics

(**drugs** for therapeutic use enabling **NMR** **diagn sis** by scalar bond)
IT 19646-38-9, p-Toluene sulfonyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(**drugs** for therapeutic use enabling **NMR** **diagnosis** by scalar bond)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L105 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:266880 HCAPLUS
DOCUMENT NUMBER: 138:276318
TITLE: **NMR** imaging **diagnostic** agents containing 17O-water
INVENTOR(S): Otsuka, Akihiro; Nakaya, Akira; Iwai, Kumiko
PATENT ASSIGNEE(S): Nihon Mediphysics Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003102698	A2	20030408	JP 2001-301681	20010928
WO 2003028769	A1	20030410	WO 2002-JP9872	20020925

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2001-301681 A 20010928
AB The agents, useful for anal. of **tissue** perfusion (e.g., blood flow), are biol. acceptable aq. solns. contg. mols. having H atom directly bonded to quadrupole nucleus and showing (a) T2 relaxation .gtoreq.0.1 s-1at.%-1 and/or (b) inhibition of change in biol. information after **bolus** dose. A soln. contg. 0.9% NaCl in H2O contg. 5 at.% H217O showed 0.17-1.1 s-1at.%-1 T2 relaxation at pH 5.0-8.0.
IC ICM A61B005-055
ICS A61K049-00; G01R033-28
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 9
ST **NMR** imaging **diagnostic** agent T2 relaxation; blood flow analysis **NMR** **diagnostic** agent; sodium chloride **NMR** imaging **diagnostic** agent
IT **Imaging agents**
(**NMR** contrast; **NMR** imaging **diagnostic** agents contg. 17O-water and biol. ions)
IT **Diagnosis**
(agents; **NMR** imaging **diagnostic** agents contg. 17O-water and biol. ions)
IT Circulation
(anal.; **NMR** imaging **diagnostic** agents contg. 17O-water and biol. ions)

IT 7440-09-7, Potassium, biological studies 7440-23-5, Sodium, biological studies 7440-70-2, Calcium, biological studies 7647-14-5, Sodium chloride, biological studies **13768-40-6**, Water-17O
RL: **DGN (Diagnostic use)**; BIOL (Biological study); USES (Uses)
(NMR imaging **diagnostic** agents contg. 17O-water and biol. ions)

L105 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:10813 HCAPLUS
DOCUMENT NUMBER: 136:66628
TITLE: Imaging methods for visualizing implanted living cells
INVENTOR(S): Moseley, Michael E.; Kucharczyk, John
PATENT ASSIGNEE(S): The Regents of the University of Minnesota, USA; The Board of Trustees of the Leland Stanford Jr. University
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002001242	A2	20020103	WO 2001-US17403	20010530
WO 2002001242	A3	20020613		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR

PRIORITY APPLN. INFO.: US 2000-606137 A 20000628

AB Cell transplantation is becoming an increasingly important method of therapy for patients. There has been no uniform methodol. or instrumentality for relatively non-invasive observation of the progression or success of the cell implantation. A method is provided herein for indicating viability of transplanted cells with a medical device that supports at least one sensing function comprising: non-destructively observing a region of a patient to where cells have been transplanted; guiding the medical device to said region of a patient using the non-destructive observation; positioning said medical device within said region of a patient using the non-destructive observation to assist in the positioning; sensing a property within said region of a patient that is indicative of cell viability or inviability; and using data from sensing said property within said region to indicate cell viability from a transplant with the region. Magnetic Resonance Imaging is a particularly useful format for non-destructive observation of the region. As an example, cell viability may indicated by a property resulting from an event selected from the group consisting of the cell activity, cell inactivity, cell growth, cell death, specific cell function, specific cell dysfunction, volumetric expansion of cell population, and volumetric decrease of cell population, while the property may be detd. with monitoring by at least one technique selected from the group consisting of proton spectroscopy, monitoring of C-13 labeled glucose, monitoring by P-31 MR spectroscopy, monitoring of local F-19 labeled metabolites, monitoring of Na-23 levels, and monitoring of 17O2 gas conversion to H217O water.

IC ICM G01R033-46
ICS A61B005-00; G01R033-563; A61B005-04; A61B005-055
CC 9-16 (Biochemical Methods)
Section cross-reference(s): 1, 8, 63
ST imaging visualizing implanted living cell
IT Optical imaging devices
(**NMR**, RF coil; imaging methods for visualizing implanted living cells)
IT Imaging
(**NMR**; imaging methods for visualizing implanted living cells)
IT Coloring materials
(Optically-active; imaging methods for visualizing implanted living cells)
IT Stress, animal
(Oxygenation; imaging methods for visualizing implanted living cells)
IT Metabolism, animal
(Phosphorous high-energy metabolites; imaging methods for visualizing implanted living cells)
IT Spectroscopy
(Proton; imaging methods for visualizing implanted living cells)
IT Electric properties
(biol.; imaging methods for visualizing implanted living cells)
IT **Imaging agents**
(contrast; imaging methods for visualizing implanted living cells)
IT Information systems
(data; imaging methods for visualizing implanted living cells)
IT Animal cell
Animal **tissue**
Cell death
Cell proliferation
Circulation
Concentration (condition)
Density
Diffusion
Electric impedance
Fluorescence
Imaging
Luminescence, bioluminescence
Materials
Medical goods
Oxidation
Temperature
Transplant and Transplantation
Volume
(imaging methods for visualizing implanted living cells)
IT Hemoglobins
Hemoglobins, oxyhemoglobins
RL: ANT (Analyte); ANST (Analytical study)
(imaging methods for visualizing implanted living cells)
IT Energy-rich phosphates
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(imaging methods for visualizing implanted living cells)
IT Brain, **disease**
(ischemia, focal; imaging methods for visualizing implanted living cells)
IT **NMR** spectroscopy
(phosphorus-31; imaging methods for visualizing implanted living cells)
IT Spin-lattice relaxation
Spin-spin relaxation

(shortening agents; imaging methods for visualizing implanted living cells)

IT 56-12-2, .gamma.-Aminobutyric acid, analysis 57-00-1, Creatine 62-49-7, Choline 107-73-3, Phosphocholine 997-55-7
RL: ANT (Analyte); ANST (Analytical study)
(imaging methods for visualizing implanted living cells)

IT 50-21-5, analysis 50-99-7, Glucose, analysis 7440-23-5, Sodium-23, analysis 7732-18-5, Water, analysis 7782-41-4D, Fluorine-19, metabolites labeled with, analysis 7782-44-7, Oxygen, analysis **13768-40-6**, Water-17O 13968-48-4, Oxygen 17, analysis 19030-38-7, Glucose, labeled with carbon 13, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(imaging methods for visualizing implanted living cells)

IT 7440-63-3, Xenon, biological studies
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(imaging methods for visualizing implanted living cells)

L105 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:690948 HCAPLUS
DOCUMENT NUMBER: 128:45418
TITLE: Strong and weak binding of water to proteins studied by **NMR** triple-quantum filtered relaxation spectroscopy of 17O-water
AUTHOR(S): Torres, Allan M.; Grieve, Stuart M.; Chapman, Bogdan E.; Kuchel, Philip W.
CORPORATE SOURCE: Department of Biochemistry, the University of Sydney, Sydney, N.S.W., Australia
SOURCE: Biophysical Chemistry (1997), 67(1-3), 187-198
CODEN: BICIAZ; ISSN: 0301-4622
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The triple-quantum filtered (TQF) spin-echo signal of 17O-water, in the presence of proteins, was analyzed to yield ests. of the no. of weakly, and strongly bound water mols. The anal. used a constrained direct iterative regression procedure with a three-state model of fast-exchange. Thus, the population size of free, weakly, and strongly bound water were detd. simultaneously. The two fractions of the bound water were estd. by using correlation time(s) estd. in other studies. Bovine serum albumin (BSA), basic pancreatic trypsin inhibitor (BPTI), lysozyme and oxyHb were studied. Of the four proteins, BSA contained the largest no. of strongly and weakly bound water mols., there being .apprx.30 of the former and .apprx.3000 of the latter under conditions of high protein concn. The correlation time of the proteins increases with their concn. in soln., and when this was taken into account for BSA the estd. no. of strongly bound water mols. did not change significantly. This NMR technique, and data anal., will probably also be useful in studies of water binding and mobility in various systems including hydrogels, protein networks, membranes, cells and **tissues**.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6, 7, 61

ST water binding protein TQF **NMR** spectrometry; triple quantum filtered relaxation **NMR** spectroscopy

IT Albumins, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(serum; strong and weak binding of water to proteins studied by **NMR** triple-quantum filtered relaxation spectroscopy of

17O-water)
IT Hydration, chemical
(strong and weak binding of water to proteins studied by NMR triple-quantum filtered relaxation spectroscopy of 17O-water)
IT Hemoglobins, oxyhemoglobins
Proteins, general, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(strong and weak binding of water to proteins studied by NMR triple-quantum filtered relaxation spectroscopy of 17O-water)
IT NMR spectroscopy
(triple-quantum filtered relaxation; strong and weak binding of water to proteins studied by NMR triple-quantum filtered relaxation spectroscopy of 17O-water)
IT 7732-18-5, Water, biological studies 9001-63-2, Lysozyme 9087-70-1, BPTI **13768-40-6**, Water-17O
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(strong and weak binding of water to proteins studied by NMR triple-quantum filtered relaxation spectroscopy of 17O-water)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L105 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:392466 HCAPLUS
DOCUMENT NUMBER: 125:142040
TITLE: Hydration of amines, diamines, polyamines and amides studied by NMR
AUTHOR(S): Okoushi, Shoichi; Moto, Tetsuhi; Ishihara, Yoshimasa; Numajiri, Haruhiko; Uedaira, Hisashi
CORPORATE SOURCE: Dep. Mater. Chem., Hosei Univ., Koganei, 184, Japan
SOURCE: Journal of the Chemical Society, Faraday Transactions (1996), 92(11), 1853-1857
CODEN: JCFTEV; ISSN: 0956-5000
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The spin-lattice relaxation times, T1, of natural abundance H21170 have been measured for aq. **solns**. of nine amines, five diamines, two polyamines and five amides, as a function of the concn. at 25.degree.C. The water-accessible surface areas of the solute mols. were calcd.. The coordination no., nh, and the rotational correlation times, .tau.ch, of water mols. around the solute mols. were estd. and compared with that of pure water .tau.c0. The value of .tau.ch/.tau.c0 = 2.02 for tert-butylamine is the largest and that of .tau.ch/.tau.c0 = 0.97 for urea the smallest obtained. The value of nh (.tau.ch/.tau.c0 - 1) was defined as the dynamic hydration no. (DHN). The partial molar vols. and the partial molar heat capacities for these homologues at infinite diln. are linearly dependent on their DHN.
CC 22-13 (Physical Organic Chemistry)
ST amine NMR hydration; diamine NMR hydration; polyamine NMR hydration; amide NMR hydration
IT Hydration, chemical
Hydration number
(dynamic; hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Homologous series
(hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Amines, properties
RL: PRP (Properties)

(hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Amides, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Molecules
(surface area; hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Amines, properties
RL: PRP (Properties)
(di-, hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Molar volume and Molecular volume
(partial, hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Heat capacity
(partial molar, hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Amines, properties
RL: PRP (Properties)
(poly-, hydration of amines, diamines, polyamines and amides examd. by NMR)
IT Magnetic relaxation
(spin-lattice, 17O; hydration of amines, diamines, polyamines and amides examd. by NMR)
IT **13768-40-6**, Water-17O
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(hydration of amines, diamines, polyamines and amides examd. by NMR)
IT 57-13-6, Urea, properties 60-35-5, Acetamide, properties 71-44-3 74-89-5, Methylamine, properties 75-04-7, Ethylamine, properties 75-31-0, Isopropylamine, properties 75-64-9, tert-Butylamine, properties 78-81-9, Isobutylamine 79-05-0, Propionamide 107-10-8, Propylamine, properties 107-15-3, 1,2-Ethanediamine, properties 109-73-9, Butylamine, properties 109-76-2, 1,3-Propanediamine 110-58-7, 1-Pentanamine 110-60-1, 1,4-Butanediamine 124-09-4, 1,6-Hexanediamine, properties 124-20-9 462-94-2, 1,5-Pentanediamine 626-97-1, Pentanamide 628-02-4, Hexanamide 13952-84-6, Sec-Butylamine
RL: PRP (Properties)
(hydration of amines, diamines, polyamines and amides examd. by NMR)

L105 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:811831 HCAPLUS
DOCUMENT NUMBER: 123:250191
TITLE: Detection of 17O by proton T1.rho. dispersion imaging
AUTHOR(S): Reddy, Ravinder; Stolpen, Alan H.; Leigh, J. S.
CORPORATE SOURCE: Dep. Radiology MMRRCC, Stellar-Chance Lab., School Medicine, University Pennsylvania, Philadelphia, PA, 19104-6100, USA
SOURCE: Journal of Magnetic Resonance, Series B (1995), 108(3), 276-9
CODEN: JMRBE5; ISSN: 1064-1866
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect of 17O-enriched water on proton T1 relaxation enhancement in aq. phantoms was examd. at high magnetic field strength. H217O produced marked enhancement of proton T1 relaxation in aq. phantoms. The method has potential applications in functional magnetic resonance imaging, particularly in the measurement of **tissue** perfusion and oxidative metab.
CC 8-9 (Radiation Biochemistry)

ST oxygen 17 **NMR** imaging phantom
IT Imaging
(**NMR**, 17O **NMR** imaging of aq. phantom)
IT **Magnetic** relaxation
(spin-lattice, 17O **NMR** imaging of aq. phantom)
IT **13768-40-6**, Water-17O
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(17O **NMR** imaging of aq. phantom)

L105 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:26749 HCAPLUS
DOCUMENT NUMBER: 120:26749
TITLE: Effects of oxygen-17-labeled water on the backbone amide proton relaxation rates of the [U-15N]FKBP/ascomycin complex
AUTHOR(S): Yu, Liping; Olejniczak, Edward T.; Fesik, Stephen W.
CORPORATE SOURCE: Pharm. Discov. Div., Abbott Lab., Abbott park, IL, 60064, USA
SOURCE: Journal of Magnetic Resonance, Series B (1993), 102(2), 218-21
CODEN: JMRBE5; ISSN: 1064-1866
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The method of C. H. Lin et al. (1991), which depends on the change in the 1H NMR relaxation rates of a biomacromol. in the presence of 17O-labeled water and which was tested on a DNA/**drug** adduct, was evaluated on the well-characterized FK506-binding protein (FKBP)/ascomycin complex by comparing the T1 and T2 relaxation times of the backbone amide protons of FKBP in the presence of 16O-labeled water vs. 17O-labeled water. Results from the FKBP/ascomycin complex are contradictory to the earlier observations of Lin et al. and suggest that their results are probably not due simply to water mols. tightly bound to the DNA/**drug** adduct.
CC 9-5 (Biochemical Methods)
Section cross-reference(s): 77
ST biopolymer bound water detection NMR spectrometry; proton magnetic relaxation protein water; FKBP ascomycin complex water magnetic relaxation
IT Water of hydration
(detn. of location of, on biomacromols. by NMR spectrometry)
IT Biopolymers
Proteins, biological studies
RL: ANST (Analytical study)
(water bound to, detn. of location of, by NMR spectrometry)
IT Proteins, specific or class
RL: ANST (Analytical study)
(FKBP (FK 506-binding protein), complexes with ascomycin, water labeled with oxygen-17 effect on backbone amide proton relaxation rates of)
IT Macromolecular compounds
RL: ANST (Analytical study)
(biol., water bound to, detn. of location of, by NMR spectrometry)
IT Magnetic relaxation
(spin-lattice, of protons of backbone amides in FK 506-binding protein-ascomycin complex)
IT Magnetic relaxation
(spin-spin, of protons of backbone amides in FK 506-binding protein-ascomycin complex)
IT **13768-40-6**, Water-17O
RL: ANST (Analytical study)
(proton relaxation rates of backbone amides of FK 506-binding protein-ascomycin complex response to)
IT 104987-12-4D, Ascomycin, complexes with FK 506-binding protein

RL: ANST (Analytical study)
(water labeled with oxygen-17 effect on backbone amide proton relaxation rates of)

L105 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:72207 HCAPLUS
DOCUMENT NUMBER: 118:72207
TITLE: **NMR** relaxation in binary aqueous mixtures of acetone and tetrahydrofuran
AUTHOR(S): Ludwig, R.; Zeidler, M. D.
CORPORATE SOURCE: Inst. Phys. Chem., RWTH, Aachen, D-5100, Germany
SOURCE: Journal of Molecular Liquids (1992), 54(4), 181-91
CODEN: JMLIDT; ISSN: 0167-7322
DOCUMENT TYPE: Journal
LANGUAGE: English
AB NMR proton relaxation rates of normal and 17O-enriched H2O and deuteron relaxation rates of D2O were measured in mixts. with acetone and THF at different **compns**. The 17O-induced proton relaxation rate was extd. and from this the rotational correlation time of H2O was detd. Using these correlation times the **compn**. dependence of the deuteron quadrupole coupling const. of H2O was derived. A strong variation was found for the system acetone-H2O, whereas little variation was obsd. for THFe-H2O.
CC 77-7 (Magnetic Phenomena)
ST **NMR** relaxation acetone THF aq mixt; quadrupole coupling water deuteron; proton relaxation oxygen 17 water; rotation correlation water acetone THF mixt
IT Quadrupole coupling
(deuteron, of water in acetone-tetrahydrofuran aq. mixts.)
IT Molecular rotation
(of water in acetone-tetrahydrofuran aq. mixts., correlation time of)
IT **Magnetic** relaxation
(spin-lattice, in acetone-tetrahydrofuran aq. mixts.)
IT 67-64-1, Acetone, properties
RL: PRP (Properties)
(nuclear spin-lattice relaxation in aq. mixts. of THF and)
IT 109-99-9, Tetrahydrofuran, properties
RL: PRP (Properties)
(nuclear spin-lattice relaxation in aq. mixts. of acetone and)
IT 7732-18-5, Water, properties
RL: PRP (Properties)
(rotational correlation time of, in acetone-tetrahydrofuran aq. mixts.)
IT 7789-20-0, Water-d2
RL: PRP (Properties)
(spin-lattice relaxation of deuteron in mixts. of acetone and THF and)
IT **13768-40-6**, Water-17O
RL: PRP (Properties)
(spin-lattice relaxation of proton in mixts. of acetone and THF and)

L105 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:210372 HCAPLUS
DOCUMENT NUMBER: 116:210372
TITLE: The stability of proton T2 effects of oxygen-17-water in experimental cerebral ischemia
AUTHOR(S): Hopkins, A. L.; Lust, W. D.; Haacke, E. M.; Wielopolski, P.; Barr, R. G.; Bratton, C. B.
CORPORATE SOURCE: Dep. Anat., Case West. Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Magnetic Resonance in Medicine (1991), 22(1), 167-74
CODEN: MRMEEN; ISSN: 0740-3194

DOCUMENT TYPE: Journal
LANGUAGE: English
AB The gerbil model of unilateral cerebral ischemia has been used to test the temporal and spatial stability of the magnetic resonance imaging (MRI) T2 effects of [17O]water (H217O). Following unilateral carotid ligation, symptomatic animals were given a single large i.p. injection of H217O and the distribution and stability of the brain T2 effects were followed with a spin-echo sequence. In contrast to the ischemic area, the perfused **tissue** shows a marked and prolonged loss in intensity with little evidence of diffusion of the T2 effect of 17O into the ischemic **tissue**.
CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 14
ST brain ischemia NMR imaging; oxygen 17 water imaging brain ischemia
IT Imaging
(**NMR**, of brain ischemia, with oxygen-17-water)
IT Brain, **disease**
(ischemia, **NMR** imaging of, with oxygen-17-water)
IT **Magnetic** relaxation
(spin-spin, of brain ischemia, using oxygen-17-water, stability of, imaging in relation to)
IT **13768-40-6**, Water-17O
RL: BIOL (Biological study)
(**NMR** imaging with, of brain ischemia)

L105 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:406771 HCAPLUS
DOCUMENT NUMBER: 113:6771
TITLE: Natural-abundance oxygen-17 **magnetic** relaxation in aqueous **solutions** of apolar **amino acids** and glycine peptides
AUTHOR(S): Ishimura, Miyuki; Uedaira, Hisashi
CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1990), 63(1), 1-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The spin-lattice relaxation times, T1, of H217O have been measured for the aq. **solns**. of 11 apolar **amino acids** and 5 glycine peptides, as a function of the concn. at 25.degree.. The coordination nos., nh, and the rotational correlation times, .tau.ch, of water mols. around the **amino acids** and peptides were estd. and compared with that of pure water, .tau.c0. The value of .tau.ch/.tau.c0 = 1.87 for norleucine is the largest, while those of .tau.c/.tau.c0 for glycine peptides are almost the same, 1.2. The value of nh(.tau.ch/.tau.c0-1) was defined as the dynamic hydration no. (DHN). The DHN showed a good correlation with several physicochem. properties, such as the mol. wts., partial molar volumes, adiabatic compressibilities, heat capacities, B-coeffs. of the activity coeff., and limiting diffusion coeffs. of **amino acids** and glycine peptides in aq. **solns**.
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22
ST dynamic **hydration number amino acid** ; glycine oligomer dynamic **hydration number**; oxygen 17 **NMR** relaxation **amino acid**; thermodn structure property relationship
IT **Hydration number**

(dynamic, of **amino acids** and glycine oligomers, by oxygen-17 **magnetic** relaxation of aq. **solns**.)

IT **Amino acids**, properties
RL: PRP (Properties)
(oxygen-17 **magnetic** relaxation of **soln**. of, thermodn. properties in relation to)

IT **Magnetic** relaxation
(spin-lattice, of oxygen-17 in aq. **solns**. of **amino acids** and glycine oligomers, thermodn. properties in relation to)

IT Molecular structure-property relationship
(thermodn., of **amino acids** and glycine oligomers, by oxygen-17 **magnetic** relaxation of aq. **solns**.)

IT 56-12-2, .gamma.-Aminobutyric acid, properties 56-40-6, Glycine, properties 56-41-7, L-Alanine, properties 61-90-5, L-Leucine, properties 72-18-4, Valine, properties 73-32-5, Isoleucine, properties 107-95-9, .beta.-Alanine 327-57-1, Norleucine 541-48-0, .beta.-Aminobutyric acid 556-33-2, Triglycine 556-50-3, Diglycine 637-84-3, Tetraglycine 2835-81-6, .alpha.-Aminobutyric acid 3887-13-6, Hexaglycine 6600-40-4, Norvaline 7093-67-6, Pentaglycine
RL: PRP (Properties)
(oxygen-17 **magnetic** relaxation of **soln**. of, thermodn. properties in relation to)

IT **13768-40-6**, Water-17O
RL: PROC (Process)
(spin-lattice relaxation of, in the presence of **amino acids** and glycine oligomers, thermodn. properties in relation to)

L105 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:36214 HCAPLUS
DOCUMENT NUMBER: 110:36214
TITLE: Oxygen-17 contrast agents. Fast imaging techniques
AUTHOR(S): Hopkins, Amos L.; Haacke, E. Mark; Barr, Richard G.; Tkach, Jean
CORPORATE SOURCE: Dep. Anat., Case Western Reserve Univ., Cleveland, OH, USA
SOURCE: Investigative Radiology (1988), 23(Suppl. 1), S240-S242
CODEN: INVRAV; ISSN: 0020-9996
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Under physiol. conditions, the stable isotope 17O, in the form of H217O, lowers the proton T2 of blood, cerebrospinal fluid, **tissues**, and whole organisms. With magnetic resonance imaging the resulting changes in intensity can be detected using spin-echo pulse sequences, but much greater sensitivity is achieved in a fraction of the time with a steady-state free precession sequence such as FISP (fast imaging with steady precision). With this sequence, it is possible to detect levels of .gtoreq.0.4% 17O water in .ltoreq.53 s.

CC 8-9 (Radiation Biochemistry)

ST **magnetic** resonance imaging oxygen 17

IT Cerebrospinal fluid
Kidney
(**magnetic** resonance imaging of, oxygen-17 contrast agents for)

IT Blood
Blood plasma
(**magnetic** spin-spin relaxation of, oxygen-17 as contrast agent for, imaging in relation to)

IT Albumins, properties
RL: PRP (Properties)
(**magnetic** spin-spin relaxation of, oxygen-17 as contrast agent for, imaging in relation to)
IT Tomography
(**NMR**, of **organs** and **tissues**, oxygen-17 contrast agents for)
IT **Magnetic** relaxation
(spin-spin, imaging by, of **organs** and **tissues**, oxygen-17 contrast agents for)
IT **13768-40-6**, Water-17O 13968-48-4, Oxygen-17, biological studies
RL: BIOL (Biological study)
(contrast agent, for **NMR** imaging of **organs** and **tissues**)

L105 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1987:403416 HCAPLUS
DOCUMENT NUMBER: 107:3416
TITLE: Oxygen-17 compounds as potential **NMR** T2 contrast agents: enrichment effects of 17O-water on protein solutions and living **tissues**
AUTHOR(S): Hopkins, A. L.; Barr, R. G.
CORPORATE SOURCE: Dep. Dev. Genet. Anat., Case Western Reserve Univ., Cleveland, OH, 44106, USA
SOURCE: Magnetic Resonance in Medicine (1987), 4(4), 399-403
CODEN: MRMEEN; ISSN: 0740-3194
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The isotopic enrichment of solns., living **tissues**, and organisms with 17O in the form of H217O shortens their proton NMR transverse relaxation times (T2) and produces changes in NMR image intensity. The transverse relaxation rate (1/T2) was linearly dependent on the H217O concn. in biol. solns. up to 5% enrichment. The longitudinal relaxation time (T1) is not affected by enrichment. Equal concns. of H217O do not produce the same magnitude of T2 change in all physiol. environments. The reasons for these differences are discussed. The results suggest that certain 17O compds. should be explored as contrast agents in magnetic resonance imaging.
CC 8-9 (Radiation Biochemistry)
ST **NMR** imaging **tissue** oxygen 17
IT Kidney
(**NMR** imaging of, oxygen-17 compds. as contrast agents for)
IT Blood
Blood plasma
Cerebrospinal fluid
(**magnetic** spin-spin relaxation time of oxygen-17 in, **NMR** imaging in relation to)
IT Albumins, properties
RL: PRP (Properties)
(**magnetic** spin-spin relaxation times in solns. of, oxygen-17 effect on, **NMR** imaging in relation to)
IT Tomography
(**NMR**, of animal **tissues**, oxygen-17 compds. as contrast agents for)
IT **Magnetic** relaxation
(spin-spin, imaging by, of animal **tissues**, oxygen-17 compds. as contrast agents for)
IT **13768-40-6** 13968-48-4, Oxygen-17, properties
RL: BIOL (Biological study)
(**magnetic** spin-spin relaxation time in protein solns. and

tissues response to, **NMR** imaging in relation to)

L105 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1987:511880 HCAPLUS
DOCUMENT NUMBER: 107:111880
TITLE: Proton transverse relaxation rate of oxygen-17-enriched water
AUTHOR(S): Yeung, Hong N.; Lent, Arnold H.
CORPORATE SOURCE: Technicare Corp., Solon, OH, 44139, USA
SOURCE: Magnetic Resonance in Medicine (1987), 5(1), 87-92
CODEN: MRMEEN; ISSN: 0740-3194
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Proton transverse relaxation rates of 17O-enriched water at pH in the neutral range were detd. with isotopic **compns**. of 17O varying from natural abundance to 5%. S. Meiboom's (1961) account of the proton 1/T2 caused by the scalar interaction between the proton and 17O is generalized to accommodate new data. The generalized formulation covers 17O enrichment above the limit to which Meiboom and his coworker constrained all their work.
CC 8-9 (Radiation Biochemistry)
ST **magnetic** relaxation oxygen 17 water; imaging **NMR** **tissue** oxygen 17
IT Cerebrospinal fluid
(**NMR** imaging of, oxygen-17-enriched water spin-spin **magnetic** relaxation in relation to)
IT Tomography
(**NMR**, of animal **tissues**, oxygen-17-enriched water spin-spin **magnetic** relaxation in relation to)
IT **Magnetic** relaxation
(spin-spin, of oxygen-17-enriched water, **tissue** imaging in relation to)
IT **13768-40-6**, Water-17O
RL: BIOL (Biological study)
(**magnetic** relaxation of, spin-spin, **tissue** imaging in relation to)

=> d ibib abs 14-23

L105 ANSWER 14 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2002-590607 [63] WPIX
DOC. NO. NON-CPI: N2002-468674
DOC. NO. CPI: C2002-167066
TITLE: Identifying a differentially expressed protein in two different samples, useful for rapid identification of marker or target proteins that can be applied in the study of e.g. **drug** toxicity, by performing inverse labeling of proteins.
DERWENT CLASS: B04 J04 K08 S03
INVENTOR(S): FU, E W; MA, Z; QUINN, D F; WANG, Y K
PATENT ASSIGNEE(S): (FUEW-I) FU E W; (MAZZ-I) MA Z; (QUIN-I) QUINN D F; (WANG-I) WANG Y K; (NOVS) NOVARTIS AG; (NOVS) NOVARTIS-ERFINDUNGEN VERW GES MBH
COUNTRY COUNT: 87
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2002052271	A2	20020704	(200263)*	EN	57

RW: AT BE CH CY DE DK EA ES FI FR GB GR IE IT LU MC NL PT SE TR
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
DM DZ EC EE ES FI GB GD GE GH HR HU ID IL IN IS JP KE KG KP KR KZ
LC LK LT LU LV MA MD MK MN MX NO NZ OM PH PL PT RO RU SE SG SI SK
TJ TM TN TR TT UA US UZ VN YU ZA ZW
US 2002090652 A1 20020711 (200263)

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2002052271 A2		WO 2001-EP15228	20011221
US 2002090652 A1	Provisional	US 2000-257559P	20001222
	Provisional	US 2001-332965P	20011119
		US 2001-16627	20011210

PRIORITY APPLN. INFO: US 2001-332965P 20011119; US 2000-257559P 20001222; US 2001-16627 20011210

AN 2002-590607 [63] WPIX

AB WO 200252271 A UPAB: 20021001

NOVELTY - Identifying a differentially expressed protein in two different samples containing a population of proteins comprises performing inverse labeling of proteins.

DETAILED DESCRIPTION - The method of identifying a differentially expressed protein in two different samples containing a population of proteins comprising:

(a) providing two equal protein pools from each of a reference sample and an experimental sample;

(b) labeling the protein pools with a substantially chemically identical isotopically different protein labeling reagent for proteins, where one pool from each of the reference and experimental pools is labeled with an isotopically heavy protein labeling reagent to provide an isotopically heavy-labeled reference and experimental pools, while the remaining reference and experimental pools are labeled with an isotopically light protein labeling reagent to provide an isotopically light-labeled reference and experimental pools;

(c) combining the isotopically light-labeled reference pool with the isotopically heavy-labeled experimental pool to provide a first protein mixture;

(d) combining the isotopically heavy-labeled reference pool with the isotopically light-labeled experimental pool to provide a second protein mixture;

(e) detecting the labeled proteins from each of the two mixtures; and

(f) comparing the labeling pattern obtained for the labeled proteins in the first and second mixtures, where an inverse labeling pattern of a protein in the second mixture compared with the labeling pattern of the protein in the first mixture is indicative of the differentially expressed protein in the two different samples.

USE - The method for performing protein labeling for comparative proteomics called inverse labeling is useful for the rapid identification of marker or target proteins. Comparative analysis of protein profiles from normal and disease states, with or without **drug** treatment, can facilitate the systematic studies of proteins involved in any biological system or disease, revealing new insights into disease mechanism, identifying new targets, providing information on **drug** -action mechanisms and toxicity, or identifying surrogate markers.

ADVANTAGE - The new method of inverse labeling of proteins provides rapid, high throughput, sensitive, reliable and unambiguous identification of various classes of differentially expressed proteins.

Dwg.0/12

L105 ANSWER 15 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2001-355363 [37] WPIX
DOC. NO. NON-CPI: N2001-258219
DOC. NO. CPI: C2001-110129
TITLE: Chemical screening of various chemicals for biological or other activity, by performing assay in which chemical(s) and/or entities are present in mixture to produce outcome, applying static magnetic field, and evaluating.
DERWENT CLASS: B04 J04 S01 S03
INVENTOR(S): STAR-LACK, J M; SUGARMAN, J H
PATENT ASSIGNEE(S): (GLAX) GLAXO GROUP LTD; (GLAX) GLAXO WELLCOME INC
COUNTRY COUNT: 91
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2001033257	A1	20010510	(200137)*	EN	35
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TZ UG ZW					
W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW					
AU 2001013558	A	20010514	(200149)		
US 6307372	B1	20011023	(200165)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001033257	A1	WO 2000-US29982	20001031
AU 2001013558	A	AU 2001-13558	20001031
US 6307372	B1	US 1999-432492	19991102

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001013558	A Based on	WO 200133257

PRIORITY APPLN. INFO: US 1999-432492 19991102
AN 2001-355363 [37] WPIX
AB WO 200133257 A UPAB: 20010704
NOVELTY - A screening method comprising:
(a) performing an assay where chemical(s) and/or entities are present in a mixture to produce an outcome in a plate having a plurality of wells;
(b) applying a static magnetic field (Bo) to the mixture;
(c) applying RF magnetic pulse(s) to the mixture; and
(d) measuring and evaluating resulting FID or echo signals to evaluate the outcome of the assay.
DETAILED DESCRIPTION - A screening method comprising:
(a) providing a plate having a plurality of wells;
(b) performing an assay in which one or more chemicals and/or entities are present in a mixture to produce an outcome, and where the assay is performed in at least some of the wells of the plate;
(c) applying a static magnetic field (Bo) to the mixture;
(d) applying RF magnetic pulse(s) to the mixture; and
(e) measuring and evaluating resulting FID or echo signals to

evaluate the outcome of the assay.

INDEPENDENT CLAIMS are also included for;

(1) A method of screening comprising: (a) providing a plate having a plurality of wells; (b) combining a test compound with another chemical and/or entity to form a mixture, where the mixture is held within at least one of the wells of the plate, and where the test compound causes a detectable nuclear magnetic resonance signal to be produced that is dependent on the amount of interaction of the test compound with the mixture; (c) applying a static magnetic field (Bo) to the mixture; (d) applying one or more RF magnetic pulses to the mixture; and (e) measuring and evaluating resulting FID or echo signals to obtain information as to whether the test compound is biologically active in the mixture;

(2) A method of screening comprising: (a) providing a plurality of plates that each include multiple wells; (b) introducing a chemical and/or entity into at least some of the wells of each plate; (c) introducing a test compound into wells containing the chemical and/or entity; (d) stacking the plates on top of each other; and (e) inserting the plates into a nuclear magnetic resonance device and screening for any biologically active test compounds;

(3) Multiwell plate comprising: (a) a plate body having a plurality of wells; (b) at least one RF coil disposed within the plate body; and (c) a connector that is adapted to coupled to RF coil to a magnetic resonance imaging system; and

(4) A multiwell plate comprising a plate body having a plurality of wells, where the plate body is constructed of a material selected from a group of materials with desirable magnetic susceptibility properties to minimize spatial distortions and signal losses to facilitate detection of FID signals.

USE - Chemical screening of various chemicals for biological or other activity.

ADVANTAGE - Method gives high throughput chemical screening.

DESCRIPTION OF DRAWING(S) - Figure is a schematic block diagram of a nuclear magnetic resonance system to screen chemicals.

Imaging system 22
Magnet 24
computer 26
Gradient amplifier 28
gradient coils 30
RF coils 32
Transmitter 34
Mult-well plates 36
Receiver 38
Digitizer 40
Monitor 42
Dwg.2/12

L105 ANSWER 16 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2001-300472 [31] WPIX
DOC. NO. CPI: C2001-092328
TITLE: New **microcluster** liquid, useful for delivering hydration, oxygenation or nutritional agents or medications, produced by subjecting liquid to cavitation and reduced pressure.
DERWENT CLASS: B07
INVENTOR(S): HOLLOWAY, M A; HOLLOWAY, W D
PATENT ASSIGNEE(S): (BIOH-N) BIO HYDRATION RES LAB INC
COUNTRY COUNT: 95
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG

WO 2001030754 A2 20010503 (200131)* EN 43
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
NL OA PT SD SE SL SZ TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CR CU CZ DE DK DM
DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC
LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE
SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
AU 2001030779 A 20010508 (200149)
BR 2000015223 A 20020618 (200249)
EP 1237578 A2 20020911 (200267) EN
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT
RO SE SI
KR 2002072276 A 20020914 (200311)
US 6521248 B1 20030218 (200317)
JP 2003514646 W 20030422 (200336) 48
CN 1399559 A 20030226 (200337)

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001030754 A2		WO 2000-US41670	20001026
AU 2001030779 A		AU 2001-30779	20001026
BR 2000015223 A		BR 2000-15223	20001026
		WO 2000-US41670	20001026
EP 1237578 A2		EP 2000-990975	20001026
		WO 2000-US41670	20001026
KR 2002072276 A		KR 2002-705363	20020426
US 6521248 B1	Provisional	US 1999-161546P	19991026
		US 2000-698537	20001026
JP 2003514646 W		WO 2000-US41670	20001026
		JP 2001-533109	20001026
CN 1399559 A		CN 2000-816223	20001026

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001030779 A	Based on	WO 200130754
BR 2000015223 A	Based on	WO 200130754
EP 1237578 A2	Based on	WO 200130754
JP 2003514646 W	Based on	WO 200130754

PRIORITY APPLN. INFO: US 1999-161546P 19991026; US 2000-698537 20001026
AN 2001-300472 [31] WPIX
AB WO 200130754 A UPAB: 20011129
NOVELTY - Producing (M1) a micro-cluster liquid comprising:
(a) subjecting a liquid to cavitation such that dissolved entrained gases in the liquid form a number of cavitation bubbles; and
(b) subjecting the liquid to reduced pressure, which causes breakage of large molecule matrices into smaller liquid molecule matrices, producing a micro-cluster liquid, is new.
DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:
(1) producing (M2) a micro-cluster liquid produced comprising:
(a) subjecting a liquid to a pressure sufficient to pressurize the liquid;
(b) emitting the pressurized liquid such that a continuous stream of

liquid is created;

(c) subjecting the continuous stream of liquid to a multiple rotational vortex having a partial vacuum pressure such that dissolved entrained gases in the liquid form a number of cavitation bubbles; and

(d) subjecting the liquid containing the cavitation bubbles to a reduced pressure, where the cavitation bubbles implode or explode causing shock waves that break large liquid molecule matrices into smaller liquid molecule matrices, thereby producing a micro-cluster liquid;

(2) a micro-cluster liquid or **water** produced by M1 or M2;

(3) a composition comprising a micro-cluster **water** having a conductivity of about 3.0 - 4.0 micromhos/cm;

(4) a composition comprising a micro-cluster **water** having a Fourier transform infrared (FTIR) spectrophotometric pattern comprising a major sharp feature at about 2650 wave numbers;

(5) a composition comprising a micro-cluster **water** having a vapor pressure between 40 - 70 degrees C as determined by thermogravimetric analysis;

(6) a composition comprising a micro-cluster **water** having an **170** nuclear magnetic resonance (NMR) peak shift of at least about +30 Hertz relative to reverse osmosis **water**; and

(7) modulating a cellular performance comprising contacting a cell with a micro-cluster **water**.

USE - The **microcluster water** is used to deliver hydration, oxygenation, or agents, such as nutritional agents or medications.

ADVANTAGE - The **microcluster water** increases overall cellular performance and exchanging liquids in the cell within minutes of consumption.

Dwg.0/7

L105 ANSWER 17 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2002-017002 [02] WPIX
CROSS REFERENCE: 1998-610081 [51]; 2001-181394 [08]
DOC. NO. NON-CPI: N2002-013679
DOC. NO. CPI: C2002-004714
TITLE: Isotopically modified topical composition for improving skin appearance and texture, comprises cosmetic material mixed with liquid light transport modifier.
DERWENT CLASS: B06 D21 P34 S05
INVENTOR(S): BERRY, M J; YAVITZ, E Q
PATENT ASSIGNEE(S): (NATU-N) NATURAL VISION CENT INC
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
US 6312450	B1	20011106	(200202)*		9

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 6312450	B1 CIP of	US 1997-858967	19970520
		US 1999-379183	19990823

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 6312450	B1 CIP of	US 6009876

PRIORITY APPLN. INFO: US 1999-379183 19990823; US 1997-858967 19970520
AN 2002-017002 [02] WPIX
CR 1998-610081 [51]; 2001-181394 [08]
AB US 6312450 B UPAB: 20020109
NOVELTY - An isotopically modified topical composition, comprising a mixture of cosmetic or cosmeceutical material, and a liquid light transport modifier, is new. The light transport modifier is readily absorbed by an epidermal layer of mammalian skin to permit passage of infrared energy through the epidermal layer at reduced energy absorption.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) using infrared energy to improve the appearance of skin of an individual comprising:

(a) selecting an isotopically modified substance that permits passage of a desired radiation in the infrared region through the epidermis;

(b) applying the isotopically modified substance to an area of the epidermis; and

(c) heating the papillary dermis layer between the epidermis and the reticular dermis at the area in order to stimulate the release of factors that promote new collagen growth; and

(2) improving the effectiveness of a cosmetic or cosmeceutical composition, comprising:

(a) providing the cosmetic or cosmeceutical composition; and

(b) isotopically modifying at least one of the chemical elements contained in the cosmetic or cosmeceutical composition to alter the energy absorption characteristics and pharmacokinetic properties of the composition.

USE - For improving the appearance and texture of individual's skin epidermis.

ADVANTAGE - The composition reduces absorption of certain types of electromagnetic energy that strike the epidermis. The light transport modifier is designed to displace naturally occurring **water** within that portion, thus resulting in a reduced heat buildup in that portion. The epidermis remains intact with less chance of infection, decrease redness and loss of body fluid, and short healing time.
Dwg.0/4

L105 ANSWER 18 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2001-435706 [47] WPIX
DOC. NO. CPI: C2001-132030
TITLE: Manufacture of **water** for cosmetics, involves passing raw **water** through salt form and/or regeneration type ion exchange resin, and adjusting nuclear magnetic resonance signal half width value of **170** in **water**.
DERWENT CLASS: A91 B07 D15 D21
PATENT ASSIGNEE(S): (JAOR) ORGANO CORP
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 2001096272 A		20010410	(200147)*		4

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

JP 2001096272 A JP 1999-274078 19990928

PRIORITY APPLN. INFO: JP 1999-274078 19990928
AN 2001-435706 [47] WPIX
AB JP2001096272 A UPAB: 20010822
NOVELTY - The method involves passing raw **water** through a salt form ion exchange resin or a mixed bed of salt form and regeneration type ion exchange resin. The nuclear magnetic resonance signal half width value of **170** in **water**, is adjusted.
DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for the **water** treatment method. The salt form ion exchange resin is a carbonate and/or bicarbonate type anion exchange resin.
USE - For dilution of concentrated liquids, for drinking **water**, cosmetics, **drugs**, brewing and juice production (all claimed).
ADVANTAGE - **Water** with reduced **170** nuclear magnetic resonance signal half width value, is manufactured stably and efficiently.
Dwg.0/0

L105 ANSWER 19 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2000-255683 [22] WPIX
CROSS REFERENCE: 1998-119933 [11]
DOC. NO. CPI: C2000-077937
TITLE: Microclustered **water** useful for preparing medicaments for the treatment of e.g. **burns**, pain, diabetes and viral infections.
DERWENT CLASS: B07 C07 D16 J04
INVENTOR(S): LORENZEN, L H
PATENT ASSIGNEE(S): (LORE-I) LORENZEN L H
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
US 6033678	A	20000307	(200022)*		8

APPLICATION DETAILS:

PATENT NO	KIND		APPLICATION	DATE
US 6033678	A	CIP of	US 1990-463988	19900112
		Cont of	US 1991-670032	19910315
		Cont of	US 1992-990357	19921215
		Cont of	US 1994-208799	19940309
			US 1997-984777	19971204

FILING DETAILS:

PATENT NO	KIND		PATENT NO
US 6033678	A	Cont of	US 5711950

PRIORITY APPLN. INFO: US 1991-670032 19910315; US 1990-463988 19900112; US 1992-990357 19921215; US 1994-208799 19940309; US 1997-984777 19971204
AN 2000-255683 [22] WPIX
CR 1998-119933 [11]
AB US 6033678 A UPAB: 20000508

NOVELTY - A process for producing microclustered **water** comprising boiling **water**, passing the steam across a magnetic field, condensing the steam and adding a stabilizer and pressure to the condensed steam, is new.

DETAILED DESCRIPTION - A process for producing microclustered **water** comprises:

(a) boiling **water**;

(b) passing the steam across a magnetic field;

(c) condensing the steam at a temperature greater than 0 deg. C in the presence of light in the far infra-red to ultraviolet spectrum range to produce condensed steam;

(d) adding a stabilizer (metasilicate salt) and less than 1% of a dietary supplement template;

(e) exposing the condensed steam to a pressure greater than 1 atmosphere; and

(f) depressurizing the condensed steam to produce the microclustered **water**.

The microclustered **water** produces an **170** nuclear magnetic resonance (NMR) signal less than 115 Hz, has a conductivity of at least 3.7 psi s/cm and a surface tension of less than 61 dynes/cm.

USE - The microclustered **water** provides a means of treating abnormal states in a living organism by using a template which has activity in treating the abnormal state. The method is especially useful for treating **burns**, pain, diabetes and viral infections.

Dwg.0/2

L105 ANSWER 20 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2000-658426 [64] WPIX
DOC. NO. CPI: C2000-199453
TITLE: New **liposome**, used in e.g. cosmetics and medicines comprises object substance and amphoteric compound e.g. phospholipid.
DERWENT CLASS: B04 D21
PATENT ASSIGNEE(S): (HATT-I) HATTORI T
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 2000229815	A	20000822	(200064)*		8

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2000229815	A	JP 1999-28910	19990205

PRIORITY APPLN. INFO: JP 1999-28910 19990205
AN 2000-658426 [64] WPIX
AB JP2000229815 A UPAB: 20001209

NOVELTY - A **liposome** (I), obtained by mixing **water** having 90 Hz or less of half value of **170**-NMR signal, amphoteric substance and object substance, is new.

DETAILED DESCRIPTION - A **liposome** (I), obtained by mixing **water** having 90 Hz or less of half value of **170**-NMR signal, amphoteric substance and phospholipid is new.

USE - (I) is used as material for cosmetics and medicines.

Dwg.0/0

L105 ANSWER 21 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 2000-091849 [08] WPIX
DOC. NO. NON-CPI: N2000-071931
DOC. NO. CPI: C2000-026656
TITLE: Pure **water** and preparation of pure **water** - for use in **parenteral** injections.
DERWENT CLASS: B07 D15 D21 P81 U11
PATENT ASSIGNEE(S): (HATT-I) HATTORI T
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 11333498	A	19991207	(200008)*		11

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 11333498	A	JP 1998-145319	19980527

PRIORITY APPLN. INFO: JP 1998-145319 19980527
AN 2000-091849 [08] WPIX
AB JP 11333498 A UPAB: 20000215
NOVELTY - Pure **water** having electric conductivity of up to 1 mu S/cm, preferably up to 0.2 mu S/cm, and a half value width of **170** -NMR of up to 69 Hz is new. DETAILED DESCRIPTION - An independent claim is also included for preparation of the above-claimed pure **water**, which includes (1) a process of allowing **water** to pass through a reverse osmosis membrane and (2) a process of allowing **water** to pass through an ion exchange membrane and/or an ion exchange resin. The preparation preferably includes an additional process of allowing **water** to pass through an ultrafilter; more preferably a process of magnetisation is also included.
USE - The pure **water** can be used in **parenteral** injections., eye drops, and cosmetic solutions.
ADVANTAGE - The pure **water** obtained has high activity as **water** and contains almost no impurities.
Dwg.0/1

L105 ANSWER 22 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 1998-119933 [11] WPIX
CROSS REFERENCE: 2000-255683 [19]
DOC. NO. NON-CPI: N1998-095456
DOC. NO. CPI: C1998-039353
TITLE: Preparation of micro-clustered **water** from starting **water** - by boiling **water**, passing through magnetic field, exposing to light, condensing, adding stabiliser, adding **yeast** cells or anti-viral agent, exposing to high pressure and depressurising.
DERWENT CLASS: B07 C04 C07 D15 D16 H06 J04 X25
INVENTOR(S): LORENZEN, L H
PATENT ASSIGNEE(S): (LORE-I) LORENZEN L H
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG

US 5711950	A	19980127 (199811)*	6

APPLICATION DETAILS:

PATENT NO	KIND		APPLICATION	DATE
US 5711950	A	CIP of	US 1990-463988	19900112
		Cont of	US 1991-670032	19910315
		Cont of	US 1992-990357	19921215
			US 1994-208799	19940309

PRIORITY APPLN. INFO: US 1991-670032 19910315; US 1990-463988 19900112; US 1992-990357 19921215; US 1994-208799 19940309

AN 1998-119933 [11] WPIX
CR 2000-255683 [19]
AB US 5711950 A UPAB: 20000508
Preparation of microclustered **water** from a starting **water** comprises: (a) Boiling the starting **water** to produce steam; (b) passing the steam across a magnetic field; (c) exposing the steam to light of wavelength 610 nm - 1 mm; (d) condensing the steam at a temperature > 0 deg. C, giving condensed steam; (e) adding at least one stabiliser, comprising a metasilicate salt, to the condensed steam; (f) adding **yeast** cells or an anti-viral agent, of concentration at most 1 %, to the condensed steam; (g) exposing the condensed steam to a pressure > 1 atmosphere; and (h) depressurising the condensed steam producing microclustered **water**. The microclustered **water** produces an **170** nuclear magnetic resonance (NMR) signal of < 115 Hz, has a conductivity of at least 3.7 mu s/cm, and has a surface tension of > 61 dynes/cm. Steps (e) and (f) may be reversed.
USE - The microclustered **water** product is used in medicaments for the treatment of viral infections, and in medicaments for promotion of growth of living organisms. The process can also be used to produce medicaments for treating **burns**, pain, diabetes, and also catalysts and agricultural products.
Dwg.0/2

L105 ANSWER 23 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
ACCESSION NUMBER: 1991-007934 [02] WPIX
DOC. NO. NON-CPI: N1991-006206
DOC. NO. CPI: C1991-003520
TITLE: Magnetic resonance **tomography** and localised spectroscopy - has gp. of impulse sequences, contrast chemicals and data analysis to improve resolution.
DERWENT CLASS: B02 E12 J04 P31 S01 S03 S05 T01
INVENTOR(S): KIMMICH, R; ROMMEL, E
PATENT ASSIGNEE(S): (KIMM-I) KIMMICH R; (ROMM-I) ROMMEL E
COUNTRY COUNT: 1
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
DE 3919052	A	19910103	(199102)*		
DE 3919052	C2	19930624	(199325)		12

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

DE 3919052	A	DE 1989-3919052	19890610
DE 3919052	C2	DE 1989-3919052	19890610

PRIORITY APPLN. INFO: DE 1989-3919052 19890610
AN 1991-007934 [02] WPIX
AB DE 3919052 A UPAB: 19930928
In a nuclear magnetic resonance system, the signal acquisition period is chosen in relation to the spin locking period of the magnetising. This allows the formation or influence of picture contrast or characteristic resonance by :- (a) one of the two variables of the rotating coordinates of the spin lattice relaxation time; (b) the frequency dependence of one of these two variables. (c) The susceptibility dependence of one of these two variables.

Pref the spin locking is at or near resonance where the effective magnetic field is aligned with the magnetising to be locked or, off resonance to reduce power demand for the high frequency RF field but allow missalignment of the effective field from the field to be locked.

USE/ADVANTAGE - In nuclear magnetic resonance based **tomography**, localised relaxometry and localised spectroscopy. Previously inaccessible material characteristics can be identified. When contrast intensifiers are used the doses can be considerably reduced. Information can be taken as contrast or volume selection data measurements. No additional measurements are necessary in normal areas. @(12pp Dwg.No.1/7)@

ABEQ DE 3919052 C UPAB: 19931116
In a process for **tomography**, partic. for medical applications, based on magnetic resonance imaging, signals are recorded in a spin-locking condition or several effective frequencies and image contrast is represented by the difference between the signals. The effective field during spring-locking differs from the direction of magnetisation.

The process is used with electron paramagnetic contrast media, pref. Mn-tetra-phenyl-(p-sulphonalophenyl) -porphyrin, or diamagnetic media, pref. **17O**-enriched cpds. e.g. **water**.

ADVANTAGE - Reduced contrast media requirement, improved tissue characterisation data.
Dwg. 1/7

=> file home
FILE 'HOME' ENTERED AT 17:29:23 ON 21 JUL 2003

Search for 33S-H biological cpds


```
=> d que l10
L9        43498 SEA FILE=CAPLUS ABB=ON  PLU=ON  CYSTEINE/OBI
L10           2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L9(L)(33S OR SULFUR-33)


=> d que l18
L16       49772 SEA FILE=CAPLUS ABB=ON  PLU=ON  (THIOL OR SULFHYDR?)/OBI
L17           6 SEA FILE=CAPLUS ABB=ON  PLU=ON  L16 AND (33S OR SULFUR-33)
L18           3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L17 AND (DISULFIDES OR
                SHIELDING OR COENZYME)/TI


=> d que l21
L19       80329 SEA FILE=CAPLUS ABB=ON  PLU=ON  (THIOL OR ?SULFHYDRYL?)
L21           3 SEA FILE=CAPLUS ABB=ON  PLU=ON  L19(P)(33S OR SULFUR-33)


=> s l10 or l18 or l21
L53           6 L10 OR L18 OR L21

=> d ibib abs hitrn ind 1-6

L53  ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2003:263972  CAPLUS
DOCUMENT NUMBER:          138:398030
TITLE:                    Coenzyme B Induced Coordination of
                          Coenzyme M via Its Thiol Group to
                          Ni(I) of F430 in Active Methyl-Coenzyme M
                          Reductase
AUTHOR(S):                Finazzo, Cinzia; Harmer, Jeffrey; Bauer, Carsten;
                          Jaun, Bernhard; Duin, Evert C.; Mahlert, Felix;
                          Goenrich, Meike; Thauer, Rudolf K.; Van Doorslaer,
                          Sabine; Schweiger, Arthur
CORPORATE SOURCE:         Physical Chemistry and Organic Chemistry, ETH Zurich,
                          Zurich, CH-8093, Switz.
SOURCE:                   Journal of the American Chemical Society (2003),
                          125(17), 4988-4989
                          CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER:                American Chemical Society
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Methyl-coenzyme M reductase (MCR) catalyzes the reaction of
     methyl-coenzyme M (CH3-S-CoM) with coenzyme B (HS-CoB) to methane and
     CoM-S-S-CoB.  At the active site, it contains the nickel porphinoid F430,
     which has to be in the Ni(I) oxidn. state for the enzyme to be active.
     How the substrates interact with the active site Ni(I) has remained
     elusive.  We report here that coenzyme M (HS-CoM), which is a reversible
     competitive inhibitor to methyl-coenzyme M, interacts with its
     thiol group with the Ni(I) and that for interaction the
     simultaneous presence of coenzyme B is required.  The evidence is based on
     X-band continuous wave EPR and Q-band hyperfine sublevel correlation
     spectroscopy of MCR in the red2 state induced with 33S-labeled
     coenzyme M and unlabeled coenzyme B.
CC   7-3 (Enzymes)
ST   sulfhydryl group nickel cofactor F430 methyl coenzyme reductase
IT   Enzyme functional sites
        (active; coenzyme B induced coordination of coenzyme M via its
        thiol group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT   Sulfhydryl group
        (coenzyme B induced coordination of coenzyme M via its thiol
```

group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT Reduction
(enzymic; coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT 74-82-8, Methane, biological studies 7440-02-0, Nickel, biological studies 45127-11-5, Coenzyme M 53501-90-9, Methyl-coenzyme M 73145-13-8, Cofactor F430 104302-77-4, Coenzyme B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT 53060-41-6, Methyl-coenzyme M reductase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT 532427-72-8P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT 4263-52-9 532427-66-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
IT 532427-67-1P 532427-70-6P 532427-71-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:196114 CAPLUS
DOCUMENT NUMBER: 139:49012
TITLE: Coenzyme M binds to a [4Fe-4S] cluster in the active site of heterodisulfide reductase as deduced from EPR studies with the [33S]coenzyme M-treated enzyme
AUTHOR(S): Duin, Evert C.; Bauer, Carsten; Jaun, Bernhard; Hedderich, Reiner
CORPORATE SOURCE: Max-Planck-Institut fur Terrestrische Mikrobiologie, Marburg, D-35043, Germany
SOURCE: FEBS Letters (2003), 538(1-3), 81-84
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Heterodisulfide reductase (Hdr) from methanogenic Archaea catalyzes the reversible redn. of the heterodisulfide (CoM-S-S-CoB) of the methanogenic **thiol** coenzymes, coenzyme M (CoM-SH) and coenzyme B (CoB-SH). Upon reaction of the oxidized enzyme with CoM-SH a unique paramagnetic species is formed, which has been shown to be due to a novel type of [4Fe-4S]3+ cluster. In this work, it was addressed whether CoM-SH is directly attached to this [4Fe-4S] cluster using CoM-33SH as substrate and purified Hdr from Methanothermobacter marburgensis and Methanosarcina barkeri. With both enzymes treatment with CoM-33SH in the presence of duroquinone as an oxidant resulted in a significant broadening of the ESR spectrum as compared to CoM-SH as substrate. The signal broadening resulted from an unresolved anisotropic hyperfine coupling between the **33S** nucleus and the paramagnetic center. The results provide

compelling evidence for a direct binding of CoM-SH to the [4Fe-4S] cluster in the active site of the enzyme.

CC 7-3 (Enzymes)

ST coenzyme M binding iron sulfur cluster heterodisulfide reductase

IT Iron-sulfur clusters (protein)
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT Enzyme functional sites
(cofactor-binding; coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT 7439-89-6D, Iron, sulfur clusters 7704-34-9D, Sulfur, iron clusters 45127-11-5, Coenzyme M 104302-77-4, Coenzyme B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT 116515-35-6, Heterodisulfide reductase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:67270 CAPLUS

DOCUMENT NUMBER: 128:175199

TITLE: Ab initio calculation of NMR properties (**shielding** and electric field gradient) of **33S** in sulfur compounds

AUTHOR(S): Bagno, Alessandro

CORPORATE SOURCE: Dipartimento di Chimica Organica, Universita di Padova, Padua, 35131, Italy

SOURCE: THEOCHEM (1997), 418(2-3), 243-255
CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chem. shieldings of the S nucleus were calcd. with the GIAO method for a wide range of org. and inorg. S compds., using the 6-311++G(2d,2p) basis set. The resulting data, including calcd. elec. field gradients, are compared with other theor. results and exptl. **33S** NMR chem. shifts and line widths; with a resulting relation, joined to calcd. elec. field gradients at the nuclei, can be employed for predicting the chem. shift and line width of hitherto undetected signals. There is no general relation between **33S** shielding and electronic charge at S.

CC 77-7 (Magnetic Phenomena)

ST NMR **sulfur 33** compd; EFG **sulfur 33** ; nuclear shielding **sulfur 33**

IT Electric field gradient
GIAO (gauge invariant atomic orbital)
NMR (nuclear magnetic resonance)
Nuclear shielding
(ab initio calcn. of NMR properties of **sulfur-33** in sulfur compds.)

IT 66-27-3, Methyl methanesulfonate 67-68-5, Dimethylsulfoxide, properties 67-71-0 74-93-1, Methane **thi l**, properties 75-15-0, Carbon disulfide, properties 75-18-3, Dimethyl sulfide 75-75-2, Methanesulfonic acid 110-02-1, Thiophene 288-47-1, Thiazole 302-04-5, Thiocyanate, properties 463-58-1, Carbon oxide sulfide (COS)

556-61-6 556-64-9, Methyl thiocyanate 624-92-0, Dimethyl disulfide 666-15-9 676-84-6, Trimethyl sulfonium 758-16-7 1534-08-3 2168-84-5 2551-62-4, Sulfur fluoride (SF6) 3086-29-1, Trimethyl sulfonium chloride 3144-09-0, Methyl sulfonamide 3658-80-8, Dimethyl trisulfide 4291-05-8 4756-05-2, Thioacetone 7446-09-5, Sulfur dioxide, properties 7446-11-9, Sulfur trioxide, properties 7719-09-7, Sulfinyl dichloride 7783-06-4, Dihydrogen sulfide, properties 7783-60-0, Sulfur tetrafluoride 7791-25-5, Sulfonyl chloride 10544-50-0, Sulfur (S8), properties 14257-58-0, **Sulfur-33**, properties 14265-45-3, Sulfite 14383-50-7, Thiosulfate (S2O32-) 14808-79-8, Sulfate, properties 14844-07-6, Dithionite 15035-72-0, Hydrogen sulfide (HS1-) 15644-49-2, Carbonotrithioate 16053-58-0, Methanesulfonic acid, ion(1-) 18155-21-0, Hydrogen sulfide ion (H3S1+) 18496-25-8, Sulfide 18649-16-6, Methanesulfinamide 18683-23-3, Protonated methanethiol 21119-13-1 63056-18-8 68226-03-9 85504-08-1, Methanesulfenamide 202993-74-6, Sulfonium chloride ((SH3)Cl)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(ab initio calcn. of NMR properties of **sulfur-33** in sulfur compds.)
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1977:404800 CAPLUS
DOCUMENT NUMBER: 87:4800
TITLE: Spectroscopic methods for the study of organic **thiols**, sulfides and **disulfides**
AUTHOR(S): Jung, Guenther; Ottnad, Michael
CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep. Ger.
SOURCE: Themen Chem. Schwefels (1975), 167-91. Editor(s): Maas, Klaus. Huethig: Heidelberg, Ger. CODEN: 35HPAM
DOCUMENT TYPE: Conference; General Review
LANGUAGE: German
AB A review with 130 refs.
CC 22-0 (Physical Organic Chemistry)
ST review spectra sulfur org; **thiol** org spectra review; sulfide org spectra review; disulfide org spectra review
IT Spectra
(disulfides, sulfides, and **thiols**)
IT Circular dichroism
Electron spin resonance
Infrared spectra
Optical rotatory dispersion
Photoelectron spectroscopy
Ultraviolet and visible spectra
(of org. sulfur compds.)
IT Nuclear magnetic resonance
(of **sulfur-33**, of org. sulfur compds.)
IT Disulfides
Sulfides, properties
Thiols, properties
RL: PRP (Properties)
(spectra of)

L53 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1977:155929 CAPLUS
DOCUMENT NUMBER: 86:155929

TITLE: Nuclear coupling of **sulfur-33** and the nature of free radicals in irradiated crystals of N-acetyl-L-**cysteine**
AUTHOR(S): Hadley, Joseph H., Jr.; Gordy, Walter
CORPORATE SOURCE: Dep. Phys., Georgia State Univ., Atlanta, GA, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1977), 74(1), 216-20
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Hyperfine structure due to 33S in its natural abundance of 0.76% was measured in the ESR of free radicals produced by x-irradn. of single crystals of N-acetyl-L-cysteine at 7.7 K. Radicals produced at 77 K with principal g values of 1.990, 2.006, and 2.214 are monosulfide radicals with the 3p unpaired electron d. of 0.70 on the S. They are neg. charged mols. RCH2S-H or neutral RCH2SH2 radicals in which 90% of the spin d. of the captured electron is concd. in a d-p hybrid orbital on the S. At 300 K, these, as well as the C-centered radicals produced at the lower temp., are converted to neutral disulfide radicals RCH2SS like those obsd. in irradiated cystine.

CC 34-2 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST acetylcysteine irradn ESR; cysteine acetyl ESR

IT Radicals, properties
RL: PRP (Properties)
(ESR of sulfur-33, in irradiated crystals of acetylcysteine)

IT Electron spin resonance
(of sulfur 33, in irradiated crystals of acetylcysteine)

IT Electron spin resonance
(of sulfur-33 in irradiated crystals of acetylcysteine)

IT 616-91-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(irradn. of, free radicals in, ESR of)

IT 14257-58-0, properties
RL: RCT (Reactant); RACT (Reactant or reagent)
(nuclear coupling of, in ESR of irradiated acetylcysteine)

L53 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1976:31403 CAPLUS
DOCUMENT NUMBER: 84:31403
TITLE: Nuclear coupling of **sulfur-33** and the nature of free radicals in irradiated crystals of **cysteine** hydrochloride and N-acetyl methionine
AUTHOR(S): Hadley, Joseph H., Jr.; Gordy, Walter
CORPORATE SOURCE: Dep. Phys., Georgia State Univ., Atlanta, GA, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1975), 72(9), 3486-90
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The 33S hyperfine structure was obsd. in the ESR of irradiated crystals of cysteine.HCl.H2O and of N-acetyl-DL-methionine. In both substances the free radicals that are stable at room temp. are disulfide radicals, RCH2SS.

CC 34-2 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST ESR cysteine methionine radical; radical irradn sulfur

IT Electron spin resonance
(of cysteine hydrochloride and acetylmethionine, free radicals in relation to)

IT Spin, nuclear coupling
(of labeled sulfur, in cysteine and methionine)
IT 1115-47-5 7048-04-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(irradn. of crystals of, ESR of)

search for 14N-H biological cpds

WELLS 09/744,550

```
=> d que l57
L55        2564 SEA FILE=MEDLINE ABB=ON  PLU=ON  NITROGEN ISOTOPES/CT
L56          27 SEA FILE=MEDLINE ABB=ON  PLU=ON  L55 AND ISOLEUCINE
L57           2 SEA FILE=MEDLINE ABB=ON  PLU=ON  L56 AND 14N  2 cites

=> d que l60
L55        2564 SEA FILE=MEDLINE ABB=ON  PLU=ON  NITROGEN ISOTOPES/CT
L58         254 SEA FILE=MEDLINE ABB=ON  PLU=ON  L55 AND RELAX?
L59          78 SEA FILE=MEDLINE ABB=ON  PLU=ON  L58 AND AMINO ACID
L60           2 SEA FILE=MEDLINE ABB=ON  PLU=ON  L59 AND 14N  2 cites

=> d que l66
L55        2564 SEA FILE=MEDLINE ABB=ON  PLU=ON  NITROGEN ISOTOPES/CT
L63          77 SEA FILE=MEDLINE ABB=ON  PLU=ON  L55 AND (14N OR NITROGEN-14)
L64          20 SEA FILE=MEDLINE ABB=ON  PLU=ON  L63 AND (MAGNETIC OR NMR)
L65           5 SEA FILE=MEDLINE ABB=ON  PLU=ON  L64 AND HYDROGEN
L66           3 SEA FILE=MEDLINE ABB=ON  PLU=ON  L65 NOT (ALGAE OR AMMONIA)/TI  3 cites

=> s l57 or l60 or l66
L67           5 L57 OR L60 OR L66  5 cites total

=> d ibib abs ind 1-5

L67  ANSWER 1 OF 5     MEDLINE on STN
ACCESSION NUMBER:   1999311318      MEDLINE
DOCUMENT NUMBER:    99311318   PubMed ID: 10382309
TITLE:              Application of amino acid type-specific
                    1H- and 14N-labeling in a 2H-, 15N-labeled
                    background to a 47 kDa homodimer: potential for NMR
                    structure determination of large proteins.
AUTHOR:             Kelly M J; Krieger C; Ball L J; Yu Y; Richter G; Schmieder
                    P; Bacher A; Oschkinat H
CORPORATE SOURCE:   Forschungsinstitut fur Molekulare Pharmakologie, Berlin,
                    Germany.. kelly@fmp-berlin.de
SOURCE:             JOURNAL OF BIOMOLECULAR NMR, (1999 May) 14 (1) 79-83.
                    Journal code: 9110829. ISSN: 0925-2738.
PUB. COUNTRY:       Netherlands
DOCUMENT TYPE:      Journal; Article; (JOURNAL ARTICLE)
LANGUAGE:           English
FILE SEGMENT:       Priority Journals
ENTRY MONTH:        199907
ENTRY DATE:         Entered STN: 19990730
                    Last Updated on STN: 20000303
                    Entered Medline: 19990722
AB   NMR investigations of larger macromolecules (> 20 kDa) are
     severely hindered by rapid 1H and 13C transverse relaxation.
     Replacement of non-exchangeable protons with deuterium removes many
     efficient 1H-1H and 1H-13C relaxation pathways. The main
     disadvantage of deuteration is that many of the protons which would
     normally be the source of NOE-based distance restraints are removed. We
     report the development of a novel labeling strategy which is based on
     specific protonation and 14N-labeling of the residues
     phenylalanine, tyrosine, threonine, isoleucine and valine in a
     fully deuterated, 15N-labeled background. This allows the application of
     heteronuclear half-filters, 15N-editing and 1H-TOCSY experiments to select
     for particular magnetization transfer pathways. Results from
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investigations of a 47 kDa dimeric protein labeled in this way demonstrated that the method provides useful information for the structure determination of large proteins.

CT Check Tags: Support, Non-U.S. Gov't
Amino Acid Sequence
Amino Acids
Deuterium
Dimerization
Hydrogen
Molecular Weight
Nitrogen
Nitrogen Isotopes
Nuclear Magnetic Resonance, Biomolecular: MT, methods
*Oligopeptides: CH, chemistry
Protein Conformation
*Proteins: CH, chemistry

RN **1333-74-0 (Hydrogen)**; 7727-37-9 (Nitrogen); 7782-39-0 (Deuterium)

CN 0 (**Amino Acids**); 0 (Nitrogen Isotopes); 0 (Oligopeptides); 0 (Proteins)

L67 ANSWER 2 OF 5 MEDLINE on STN

ACCESSION NUMBER: 97144788 MEDLINE
DOCUMENT NUMBER: 97144788 PubMed ID: 8990521
TITLE: 15N conservation in the metabolic conversion of **isoleucine** to alloisoleucine in the rat.
AUTHOR: Mamer O A; Lepine F L
CORPORATE SOURCE: Biomedical Mass Spectrometry Unit, McGill University, Montreal, Quebec, Canada.
SOURCE: JOURNAL OF MASS SPECTROMETRY, (1996 Dec) 31 (12) 1382-8. Journal code: 9504818. ISSN: 1076-5174.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199702
ENTRY DATE: Entered STN: 19970305
Last Updated on STN: 19970305
Entered Medline: 19970218

AB 15N,13C6-L-**Isoleucine** was given by stomach tube to a pair of rats and the urine excreted over the following 6 h period was collected. The urinary amino acid fraction showed that the majority of the L-alloisoleucine produced from the labeled **isoleucine** was formed with the 15N label intact. This fails to support the commonly held supposition that L-**isoleucine** and L-alloisoleucine interconversion occurs through the reversible enolization of the 2-keto-3-methylvaleric acids formed by their transamination. In contrast to 15N label conservation in L-alloisoleucine, the majority of the 15N in the administered L-**isoleucine** underwent exchange with **14N**.

CT Check Tags: Animal; Male
Biotransformation
Indicators and Reagents
***Isoleucine: PK, pharmacokinetics**
Isoleucine: UR, urine
Mass Fragmentography
*Nitrogen: ME, metabolism
Nitr gen Isotopes
Organosilicon Compounds
Rats

Rats, Sprague-Dawley
Trifluoroacetic Acid: AA, analogs & derivatives
RN **73-32-5 (Isoleucine)**; 76-05-1 (Trifluoroacetic Acid); 7727-37-9 (Nitrogen); 77377-52-7 (N-methyl-N-(tert-butyldimethylsilyl)trifluoroacetamide)
CN 0 (Indicators and Reagents); 0 (Nitrogen Isotopes); 0 (Organosilicon Compounds)

L67 ANSWER 3 OF 5 MEDLINE on STN
ACCESSION NUMBER: 95005911 MEDLINE
DOCUMENT NUMBER: 95005911 PubMed ID: 7921674
TITLE: Assignment of amino acid type in 1H-15N correlation spectra by labeling with **14N**-amino acids.
AUTHOR: Shortle D
CORPORATE SOURCE: Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, Maryland 21205.
CONTRACT NUMBER: GM34171 (NIGMS)
SOURCE: JOURNAL OF MAGNETIC RESONANCE. SERIES B, (1994 Sep) 105 (1) 88-90.
Journal code: 9309764. ISSN: 1064-1866.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199411
ENTRY DATE: Entered STN: 19941222
Last Updated on STN: 19941222
Entered Medline: 19941116
CT Check Tags: Support, U.S. Gov't, P.H.S.
*Amino Acids
Amino Acids: AN, analysis
Hydrogen
***Magnetic Resonance Spectroscopy**
Micrococcal Nuclease: CH, chemistry
Nitrogen
Nitrogen Isotopes
RN **1333-74-0 (Hydrogen)**; 7727-37-9 (Nitrogen)
CN 0 (Amino Acids); 0 (Nitrogen Isotopes); EC 3.1.31.1 (Micrococcal Nuclease)

L67 ANSWER 4 OF 5 MEDLINE on STN
ACCESSION NUMBER: 94151290 MEDLINE
DOCUMENT NUMBER: 94151290 PubMed ID: 8108380
TITLE: A comparison of 15N NMR **relaxation** measurements with a molecular dynamics simulation: backbone dynamics of the glucocorticoid receptor DNA-binding domain.
AUTHOR: Eriksson M A; Berglund H; Hard T; Nilsson L
CORPORATE SOURCE: Center for Structural Biochemistry (CSB), Karolinska Institute, NOVUM, Huddinge, Sweden.
SOURCE: PROTEINS, (1993 Dec) 17 (4) 375-90.
Journal code: 8700181. ISSN: 0887-3585.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199403
ENTRY DATE: Entered STN: 19940330
Last Updated on STN: 19940330
Entered Medline: 19940322
AB The rapid motions of the backbone of the DNA-binding domain of the glucocorticoid receptor (GR DBD) have been investigated using

proton-detected heteronuclear NMR experiments on 15N-labeled protein at pH 6.0 and with a 200 psec molecular dynamics simulation of hydrated GR DBD. The experimental data were interpreted in terms of a generalized order parameter (S2) and an effective correlation time (tau e) for the internal motion of each amide bond. A back calculation, using the same model, yielded the [1H]-**14N** nuclear Overhauser effects (NOEs) and the 15N spin-lattice **relaxation** times (T1) from the simulated data. The rapid motions of the backbone turned out to be rather limited and uniform throughout the protein, with a somewhat reduced mobility in the two major alpha-helical regions and a slightly enhanced flexibility for some residues in the first zinc coordinating region. The agreement between the experimental and simulated S2-values was as good as quantitative for most of the residues, except for some residues that were subject to a more large-scale, and in the simulation thus poorly sampled, motion. Examples of such motions that were found in the simulation include jumps of the amide bond of Ile-487 between the charged oxygens of the side chain of Asp-485 and less distinct large scale motions for some of the residues in the extended regions, that were shown to give rise to noisy and/or fast decaying internal reorientational correlation functions. For these residues large differences in the simulated and experimental tau e-values were found, indicating that motions on different time scales were dominating in the experimental and simulated values. The lower (< 0.7) experimental NOEs for these residues could not be reproduced in the simulation and were shown to be a consequence of the lower tau e-values estimated in the simulation. By combining information from the simulation and the experiment a more complete picture of the motions for these residues can be obtained as is illustrated with an estimation of the jump angle and jump frequency for the amide bond of Ile-487.

CT Check Tags: Animal; Comparative Study; Support, Non-U.S. Gov't
Amino Acid Sequence
Binding Sites
*DNA: ME, metabolism
Magnetic Resonance Spectroscopy
Models, Molecular
Models, Theoretical
Molecular Sequence Data
Nitrogen Isotopes
Rats
*Receptors, Glucocorticoid: UL, ultrastructure
RN 9007-49-2 (DNA)
CN 0 (Nitrogen Isotopes); 0 (Receptors, Glucocorticoid)

L67 ANSWER 5 OF 5 MEDLINE on STN
ACCESSION NUMBER: 90234793 MEDLINE
DOCUMENT NUMBER: 90234793 PubMed ID: 2331506
TITLE: 17O- and **14N-NMR** studies of Leu-enkephalin and enkephalin-related fragments in aqueous solution.
AUTHOR: Karayannis T; Gerothanassis I P; Sakarellos-Daitsiotis M; Sakarellos C; Marraud M
CORPORATE SOURCE: Department of Chemistry, University of Ioannina, Greece.
SOURCE: BIOPOLYMERS, (1990 Feb 5) 29 (2) 423-39. Journal code: 0372525. ISSN: 0006-3525.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199006
ENTRY DATE: Entered STN: 19900706
Last Updated on STN: 19900706

Entered Medline: 19900606

AB 17O- and **14N-nmr** chemical shifts and line widths of the carboxyl and amino terminal groups of Leu-enkephalin--Tyr-Gly-Gly-Phe-[17O]Leu-Oh--and enkephalin-related fragments--[17O]Leu-OH, Phe-[17O]Leu-OH, Gly-Phe-[17O]Leu-OH, and Gly-Gly-Phe-[17O]Leu-OH--were measured in aqueous solution over the entire H pH range. Enrichment in 17O was achieved by saponification of the corresponding O-methyl esters. Ionization constants and titration shifts were obtained by nonlinear least-squares fits to one-proton titration curves. [17O]Leu-OH exhibits a profound pH-dependent solvation change on deprotonation of the carboxyl group, as shown by 17O- and **14N-nmr** line widths. In contrast, the peptides studied do not exhibit pH-dependent conformational (solvation) changes on deprotonation of the carboxyl group, and a head-to-tail intramolecular association between the ionic terminal groups should be excluded. It is shown that the peptides do not exhibit isotropic overall molecular motion and that segmental motion rather than fast internal motion influences the effective correlation times at the sites of the carboxyl oxygens and the amino nitrogen.

CT Check Tags: Comparative Study; Support, Non-U.S. Gov't

Amino Acid Sequence
*Enkephalin, Leucine
Hydrogen-Ion Concentration
Leucine
Magnetic Resonance Spectroscopy: MT, methods
Molecular Sequence Data
Molecular Weight
Nitrogen Isotopes
Oxygen Isotopes
*Peptide Fragments
Protein Conformation
Solutions
Thermodynamics
Water

RN 58822-25-6 (Enkephalin, Leucine); 61-90-5 (Leucine); 7732-18-5 (Water)
CN 0 (Nitrogen Isotopes); 0 (Oxygen Isotopes); 0 (Peptide Fragments); 0 (Solutions)

Inventor Search

WELLS 09/744,550

```
=> d his

     (FILE 'HOME' ENTERED AT 10:19:21 ON 21 JUL 2003)

     FILE 'HCAPLUS' ENTERED AT 10:19:31 ON 21 JUL 2003
L1            64 S WASHINO K?/AU
L2            37 S SHIMMURA T?/AU
L3           235 S NAKATANI A?/AU
L4           142 S FUJIMOTO C?/AU
L5          6178 S TANAKA A?/AU
L6            45 S SERI S?/AU
L7          1168 S IWAI K?/AU
L8          7854 S L1-7
L9           206 S L8 AND MAGNETIC
L10           23 S L8 AND MAGNETIC RESONANCE
L11         5768 S 17O
L12          903 S 33S
L13         9485 S 14N
L14            1 S L10 AND L11-13
                 SELECT RN L14 1

     FILE 'REGISTRY' ENTERED AT 10:22:15 ON 21 JUL 2003
L15           13 S E1-13

     FILE 'HCAPLUS' ENTERED AT 10:22:38 ON 21 JUL 2003
L16            1 S L14 AND L15
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1 cite of 13 cpds displayed

=> d ibib abs hitstr ind

L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:98382 HCAPLUS
DOCUMENT NUMBER: 132:134185
TITLE: Drugs for therapeutic use enabling nuclear **magnetic resonance** diagnosis by scalar bond
INVENTOR(S): **Washino, Komei; Shimmura, Toshiyuki ; Nakatani, Akira; Fujimoto, Chieko ; Tanaka, Akihiro; Seri, Shigemi; Iwai, Kumiko**
PATENT ASSIGNEE(S): Nihon Medi-Physics Co., Ltd., Japan
SOURCE: PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006207	A1	20000210	WO 1999-JP3970	19990723
W: AU, BR, CA, CN, KR, NO, NZ, RU, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000044491	A2	20000215	JP 1998-213050	19980728
CA 2338702	AA	20000210	CA 1999-2338702	19990723
AU 9948005	A1	20000221	AU 1999-48005	19990723
AU 758913	B2	20030403		
EP 1101498	A1	20010523	EP 1999-931523	19990723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2001000423	A	20010124	NO 2001-423	20010124

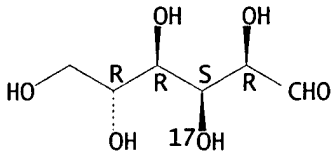
PRIORITY APPLN. INFO.: JP 1998-213050 A 19980728
WO 1999-JP3970 W 19990723

AB Drugs for therapeutic use characterized by contg. a compd. which carries in its structure at least one member selected from among -17OH, -14NH and -33SH, wherein the above **17O**, **14N** or **33S** exerts a relaxation effect on the proton bonded thereto and the relaxation effect is transported through the exchange of a proton in a vital component of a target organ or tissue by the above-mentioned proton, thus enabling detection by NMR. The effective circulation or distribution of such a physiol. acceptable therapeutic drug in the target organ or tissue in vivo where it is needed can be externally detected by the NMR method before the administration of a remedy to each patient or simultaneously therewith.

IT **257283-87-7P**, D-Glucose-3-**17O** **257283-88-8P**, D-Glucose-1-**17O**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)

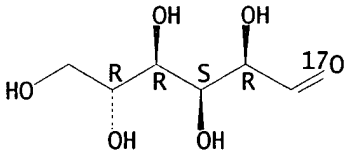
RN 257283-87-7 HCAPLUS
CN D-Glucose-3-17O (9CI) (CA INDEX NAME)

Absolute stereochemistry.

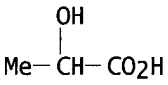


RN 257283-88-8 HCAPLUS
CN D-Glucose-1-17O (9CI) (CA INDEX NAME)

Absolute stereochemistry.

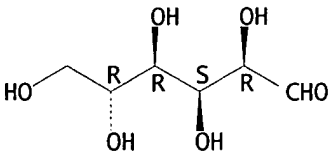


IT **50-21-5**, Lactic acid, biological studies **50-99-7**, Glucose, biological studies **4033-40-3**, N-Acetyl asparagine **7727-37-9**, Nitrogen, biological studies **12586-59-3**, Proton **13774-92-0**, Imidogen **13968-48-4**, biological studies **14257-58-0**, S-33, biological studies **15587-57-2**, Hydroxyl-17O **31713-49-2**, Mercapto-33S
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
RN 50-21-5 HCAPLUS
CN Propanoic acid, 2-hydroxy- (9CI) (CA INDEX NAME)



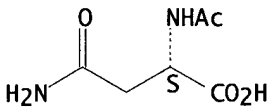
RN 50-99-7 HCAPLUS
CN D-Glucose (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4033-40-3 HCAPLUS
CN L-Asparagine, N2-acetyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 7727-37-9 HCAPLUS
CN Nitrogen (8CI, 9CI) (CA INDEX NAME)

N≡N

RN 12586-59-3 HCAPLUS
CN Proton (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 13774-92-0 HCAPLUS
CN Imidogen (8CI, 9CI) (CA INDEX NAME)

NH

RN 13968-48-4 HCAPLUS
CN Oxygen, isotope of mass 17, at. (8CI, 9CI) (CA INDEX NAME)

^{17}O

RN 14257-58-0 HCAPLUS
CN Sulfur, isotope of mass 33 (8CI, 9CI) (CA INDEX NAME)

^{33}S

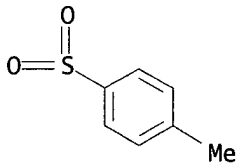
RN 15587-57-2 HCAPLUS
CN Hydroxyl-17O (7CI, 8CI, 9CI) (CA INDEX NAME)

$H^{17}O$

RN 31713-49-2 HCAPLUS
CN Mercapto-33S (8CI, 9CI) (CA INDEX NAME)

$H^{33}S$

IT **19646-38-9**, p-Toluene sulfonyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
RN 19646-38-9 HCAPLUS
CN Phenylsulfonyl, 4-methyl- (9CI) (CA INDEX NAME)



IC ICM A61K049-00
CC 8-9 (Radiation Biochemistry)
Section cross-reference(s): 63
ST radiopharmaceutical diagnosis NMR MRI scalar bond; infusion liposome radiopharmaceutical diagnosis NMR MRI
IT Diagnosis
(agents; drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT Animal tissue
Drug delivery systems
Imaging agents
NMR (nuclear **magnetic resonance**)
Organ, animal
Positron-emission tomography
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT Amino acids, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT Drug delivery systems
(infusions; drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT Drug delivery systems
(liposomes; drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT **257283-87-7P**, D-Glucose-3-**17O 257283-88-8P**, D-Glucose-1-**17O**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT **50-21-5**, Lactic acid, biological studies **50-99-7**, Glucose, biological studies **4033-40-3**, N-Acetyl asparagine **7727-37-9**, Nitrogen, biological studies **12586-59-3**, Proton **13774-92-0**, Imidogen **13968-48-4**, biological studies **14257-58-0**, S-33, biological studies **15587-57-2**, Hydroxyl-**17O 31713-49-2**, Mercapto-**33S**
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
IT **19646-38-9**, p-Toluene sulfonyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT